Atomic-Scale Engineering of the Electronic and Orbital Properties of Complex Oxides

The strong interplay between the structure and the physical properties of transition metal complex oxides allows the engineering of their functional properties by tuning their atomic scale structure. Engineering these structural properties requires precise atomic-scale synthesis control achieved using molecular beam epitaxy and advanced techniques to characterize atomic arrangements with picometer-scale resolution achieved using novel synchrotron-based diffraction techniques.

We show how this approach is applied to achieve two-dimensional electronic conductivity and an orbital polarization in nickelate heterostructures. [1, 2, 3, 4]

We use a combined synchrotron-based experimental approach and first principles theory to identify the key structural differences in LaNiO$_3$ thin films grown using molecular beam epitaxy, and relate the differences in physical structure with the measured electronic transport properties and x-ray absorption spectroscopy measurements. By identifying the general design principles which lead to breaking the degeneracy of the Nickel 3d orbitals, we design and fabricate tricomponent superlattices to control the electronic and orbital properties of rare earth nickelate compounds to control two-dimensional conductivity and to achieve a two-dimensional single band electronic surface at the Fermi energy.